Introduction to Verification and Validation

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Park City, Utah
August 6-13, 2011

Outline

- Goals of verification and validation
- Terminology
- Code verification
- Solution verification
- Aspects of validation
- Validation experiment hierarchy
- Concluding remarks

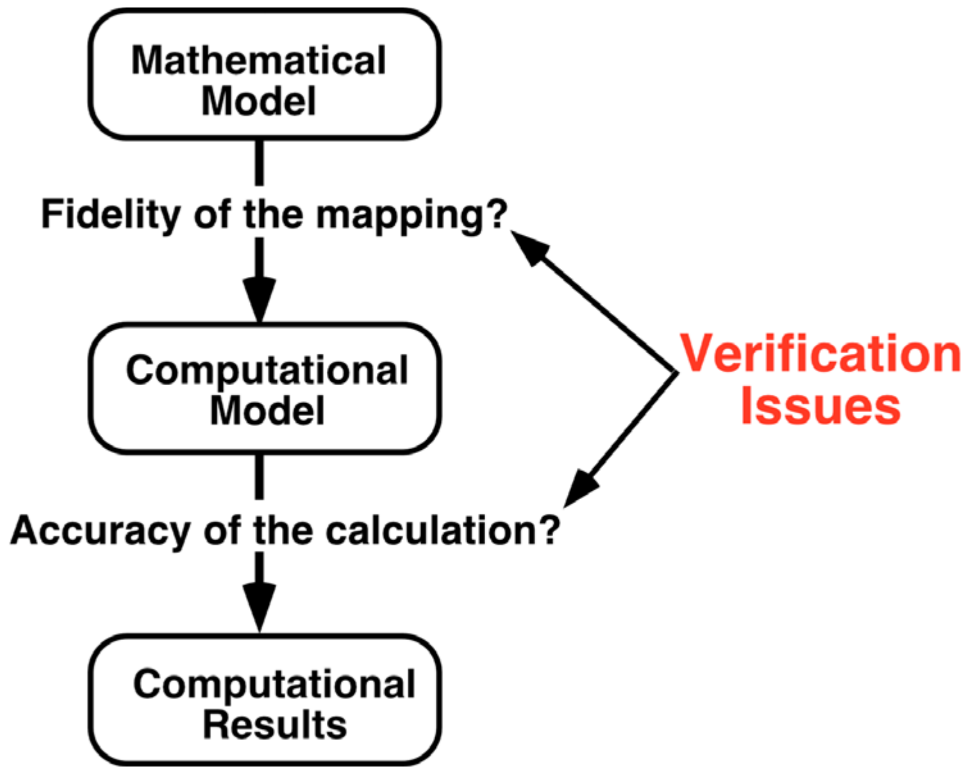
Goals of Verification and Validation

- Verification and validation are the technical tools (processes) by which simulation credibility is quantified
- Verification is the process of gathering evidence concerning the correctness of the computer code and accuracy of the numerical solution to the given mathematical model of the physics
- Validation is the process of gathering evidence concerning the accuracy and capability of the mathematical model to simulate the physics of interest
- Adequacy of verification and validation depends on:
  - Individual's view of adequate credibility
  - Consequence of the decision based on simulation

Formal Definition of Verification (DoD, AIAA, ASME)

Verification: The process of determining that a computational model accurately represents the underlying mathematical model and its solution

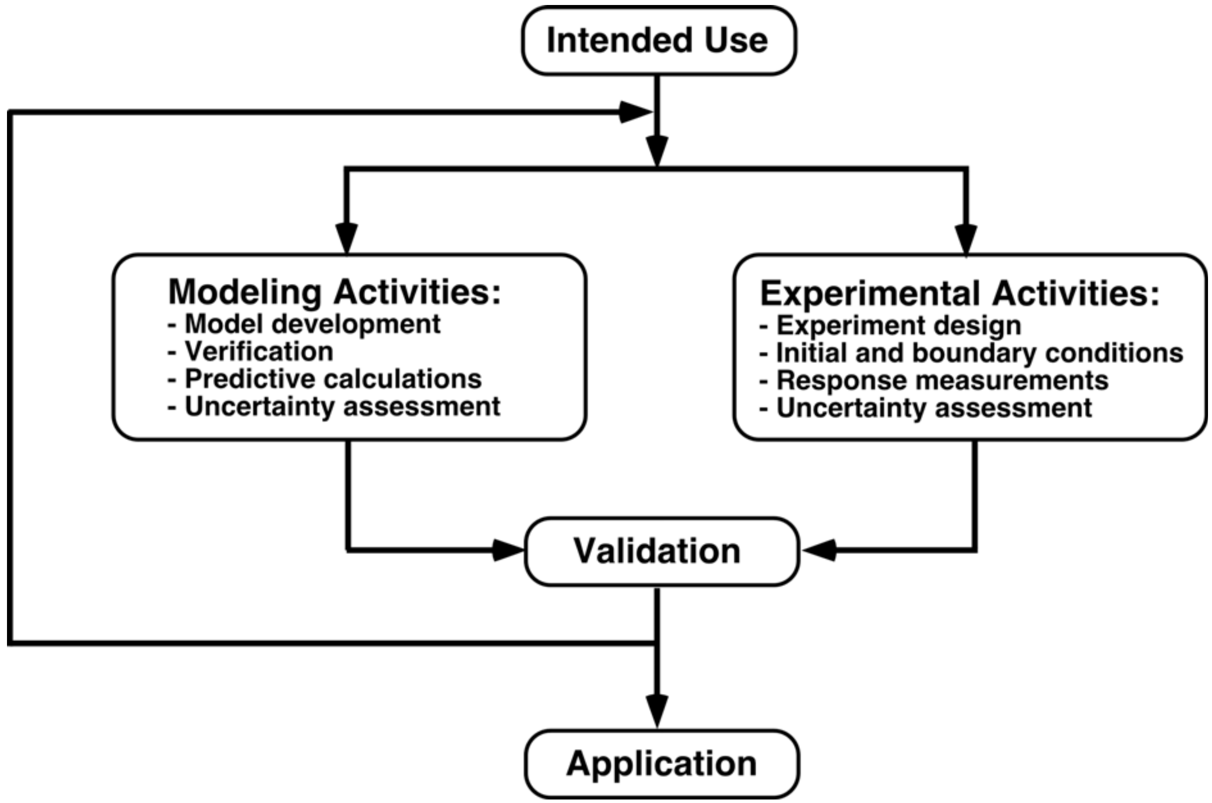
Verification deals with mathematics and software engineering



Formal Definition of Validation (DoD, AIAA, ASME)

Validation: **The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model**

Validation deals with physics



(Ref: ASME Guide, 2006)

Calibration

- When assessed accuracy of a computational result is not adequate or improved agreement is desired, then calibration is appropriate

Calibration: The process of adjusting physical modeling parameters in the computational model to improve agreement with experimental data

- Also known as: parameter estimation, model tuning, model updating

Calibration is a <u>response</u> to the assessment of model accuracy directed toward improvement of agreement with experimental data

- Calibration is critically important in many situations:
  - Calibration is commonly conducted before formal validation activities
  - Calibration of model parameters when parameters cannot be measured independently from the model

Two Types of Verification

- Verification is divided into two processes:
- Code Verification: Verification activities directed toward:
  - Finding and removing mistakes in the source code
  - Finding and removing errors in numerical algorithms
  - Improving software using software quality assurance practices
- Solution Verification: Verification activities directed toward:
  - Assuring the accuracy of input data for the problem of interest
  - Estimating the numerical solution error
  - Assuring the accuracy of output data for the problem of interest

Code Verification Processes

- **Good software engineering practices (version control, regression testing, etc.)**
- **Code *order of accuracy* testing**
  - **Demonstrate that the discretization error** $\varepsilon_h = u_h - \tilde{u}$ **reduces at proper rate with systematic mesh refinement:**

$$p = \frac{\ln\left(\varepsilon_{rh} / \varepsilon_h\right)}{\ln(r)}$$

  - **Systematic refinement requires uniform refinement over the entire domain and in all independent variables of the PDE**
- **This approach also requires an exact solution to the mathematical model**

Code Verification: Exact Solutions

Two main approaches for obtaining exact solutions to the mathematical model

- **Traditional exact solutions – given a properly posed PDE and initial / boundary conditions, find the solution**
  - **Exist only for simple models**
  - **Do not exercise the code in a general sense**
- **Method of Manufactured Solutions (MMS)**
  - **Given a PDE** $L(u) = 0$
  - **Find the modified PDE which the solution satisfies**
    - **Choose an analytic solution,** $\hat{u}$**, e.g., sinusoidal functions**
    - **Operate PDE onto the solution to give the source term:** $L(\hat{u}) = s$
    - **New PDE** $L(u) = s$ **is then numerically solved to get** u_h
  - **Discretization error can be *evaluated* as:** $\varepsilon_h = u_h - \hat{u}$

Example of MMS with Order Verification: 2D Euler Equations

2D steady-state Euler equations:

$$\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} = f_m$$

$$\frac{\partial(\rho u^2 + p)}{\partial x} + \frac{\partial(\rho u v)}{\partial y} = f_x$$

$$\frac{\partial(\rho u v)}{\partial x} + \frac{\partial(\rho v^2 + p)}{\partial y} = f_y$$

$$\frac{\partial(\rho u e_t + p u)}{\partial x} + \frac{\partial(\rho v e_t + p v)}{\partial y} = f_e$$

$$p = \rho R T, \quad e_t = \frac{1}{\gamma - 1} R T + \frac{u^2 + v^2}{2}$$

Example of MMS with Order Verification: 2D Euler Equations (contd)

Choose the form of the manufactured solution:

$$\rho(x,y) = \rho_0 + \rho_x \sin\left(\frac{a_{\rho x}\pi x}{L}\right) + \rho_y \cos\left(\frac{a_{\rho y}\pi y}{L}\right)$$

$$u(x,y) = u_0 + u_x \sin\left(\frac{a_{ux}\pi x}{L}\right) + u_y \cos\left(\frac{a_{uy}\pi y}{L}\right)$$

$$v(x,y) = v_0 + v_x \cos\left(\frac{a_{vx}\pi x}{L}\right) + v_y \sin\left(\frac{a_{vy}\pi y}{L}\right)$$

$$p(x,y) = p_0 + p_x \cos\left(\frac{a_{px}\pi x}{L}\right) + p_y \sin\left(\frac{a_{py}\pi y}{L}\right)$$

Example of MMS with Order Verification: 2D Euler Equations (contd)

Substitute the manufactured solution into the governing equations to analytically derive the source terms

- **Use symbolic manipulation tools, e.g., MatLab and Mathematica**
- **E.g., the source term for the mass conservation equation is:**

$$
\begin{aligned}
f_m = {} & \frac{a_{ux}\pi u_x}{L}\cos\left(\frac{a_{ux}\pi x}{L}\right)\left[\rho_0 + \rho_x \sin\left(\frac{a_{\rho x}\pi x}{L}\right) + \rho_y \cos\left(\frac{a_{\rho y}\pi y}{L}\right)\right] \\
& + \frac{a_{vy}\pi v_y}{L}\cos\left(\frac{a_{vy}\pi y}{L}\right)\left[\rho_0 + \rho_x \sin\left(\frac{a_{\rho x}\pi x}{L}\right) + \rho_y \cos\left(\frac{a_{\rho y}\pi y}{L}\right)\right] \\
& + \frac{a_{\rho x}\pi \rho_x}{L}\cos\left(\frac{a_{\rho x}\pi x}{L}\right)\left[u_0 + u_x \sin\left(\frac{a_{ux}\pi x}{L}\right) + u_y \cos\left(\frac{a_{uy}\pi y}{L}\right)\right] \\
& + \frac{a_{\rho y}\pi \rho_y}{L}\sin\left(\frac{a_{\rho y}\pi y}{L}\right)\left[v_0 + v_x \cos\left(\frac{a_{vx}\pi x}{L}\right) + v_y \sin\left(\frac{a_{vy}\pi y}{L}\right)\right]
\end{aligned}
$$

Example of MMS with Order Verification: 2D Euler Equations (contd)

Discretize and solve on multiple meshes (uniform)

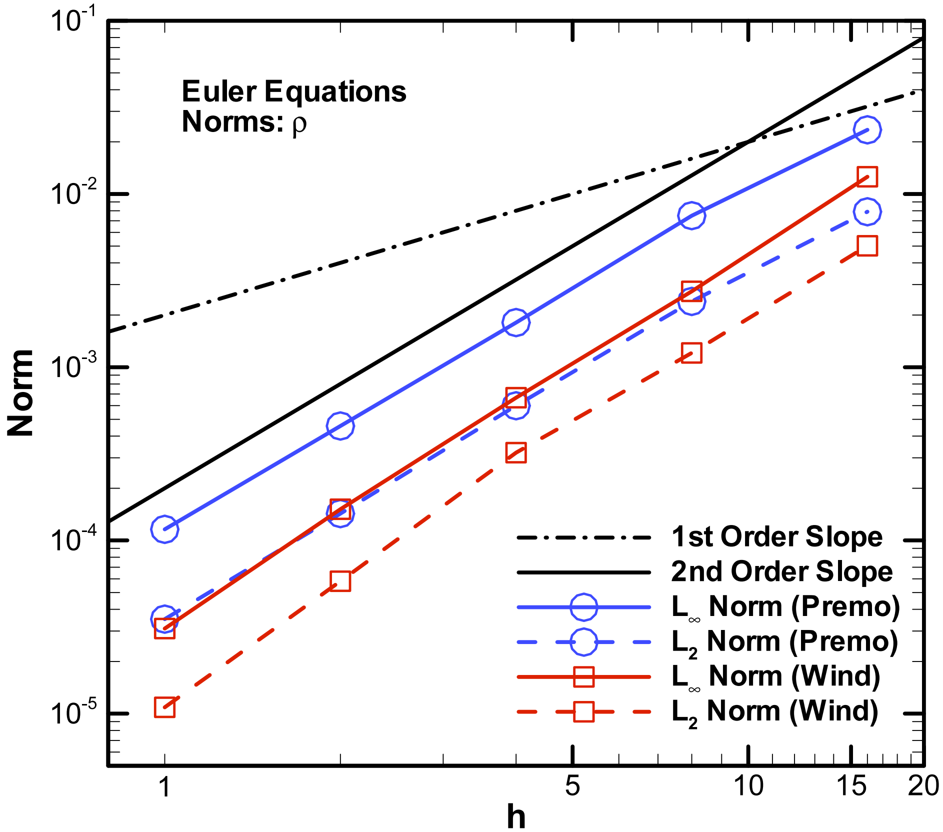
Mesh Name	Mesh Nodes	Grid Spacing, *h*
Mesh 1	129 x 129	1
Mesh 2	65 x 65	2
Mesh 3	33 x 33	4
Mesh 4	17 x 17	8
Mesh 5	9 x 9	16

- **Coarser meshes found by eliminating every other grid line in each direction from the fine mesh (*r* = 2)**
- **Grid spacing is normalized by the fine mesh spacing**

$$h_k = \frac{\Delta_k}{\Delta_1}, \quad \Delta = \Delta x = \Delta y$$

Example of MMS with Order Verification: 2D Euler Equations (contd)

Global discretization error in numerical solutions



L_∞ Norm:

$$\left\|\varepsilon_h\right\|_\infty = \max\left|u_n - \widetilde{u}_n\right|$$

L_2 Norm:

$$\left\|\varepsilon_h\right\|_2 = \left(\frac{1}{N}\sum_{n=1}^{N}\left|u_n - \widetilde{u}_n\right|^2\right)^{1/2}$$

- $\widetilde{u}$ **from manuf. solution**
- ***n* = nodes**
- **Second-order accuracy is demonstrated**

Solution Verification

- **In code verification, the exact solution to the PDEs was known and used to *evaluate* the discretization error**
- **In solution verification, the various sources of numerical error must be *estimated***
  - **Round-off error**
  - **Iterative error**
  - **Discretization error**

Iterative Error

Iterative error can be generally defined as the difference between the current approximate iterative solution and the exact solution to the equations

- **It occurs any time an iterative method is used to solve algebraic equations**
- **For scientific computing:**
  - **The system of algebraic equations usually arises from the discretization of a mathematical model**
  - **The exact solution in the above definition is the exact solution to the *discrete equations* (not the PDEs)**

Discretization Error

Discretization Error (DE) is the difference between the exact solution to the discrete equations and the exact solution to the partial differential equations (PDEs)

$$\varepsilon_h = u_h - \widetilde{u}$$

- DE is the numerical approximation error due to the mesh and/or time step used in the numerical scheme
- DE comes from the interplay between the numerical scheme, the mesh resolution, the mesh quality, and the solution behavior

Solution Verification: Classification of DE Estimators

Of the sources of numerical error, discretization error (DE) is usually the largest and most difficult to estimate

- **Type 1: DE estimators based on higher-order estimates of the exact solution to the PDEs (post-process the solution)**
  - **Richardson extrapolation**
  - **Order refinement methods**
  - **Finite element recovery methods**
- **Type 2: Residual-based methods (include additional information about problem being solved)**
  - **DE transport equations**
  - **Finite element residual methods**
  - **Defect correction methods**
  - **Adjoint methods for SRQs**

Generalized Richardson Extrapolation

- **DE expansion for a formally *p*th order scheme:**

$$\varepsilon_h = u_h - \widetilde{u} = g_p h^p + g_{p+1} h^{p+1} + g_{p+2} h^{p+2} + \ldots$$

- **Uses solutions on two meshes systematically-refined by the factor** $r = h_{\text{coarse}} / h_{\text{fine}}$ **where** $h_{\text{coarse}} = rh_{fine} = rh$

- **Assuming H.O.T. are small, an estimate of the exact solution is given by:**

$$\overline{u} = u_h + \frac{u_h - u_{rh}}{r^p - 1}$$

- $\overline{u}$ **can be used to provide the DE estimate**

$$\overline{\varepsilon}_h = u_h - \overline{u}$$

Richardson Extrapolation (cont'd)

Advantages

- **Can be applied as a post-processing step**
- **Independent of the type of numerical scheme (finite difference, finite volume, finite element)**
- **Applies to dependent variables and any global quantities**

Disadvantages

- **Requires solutions on two systematically-refined mesh levels**
- **<u>Both</u> numerical solutions must be asymptotic for the error estimates to be reliable**

All solution error estimates require the solution to be asymptotic

Goals of Validation

Tactical goal of validation: Identification and quantification of uncertainties and errors in the computational model and in the experimental measurements

Strategic goal of validation: Increase confidence in the quantitative predictive capability of the computational model

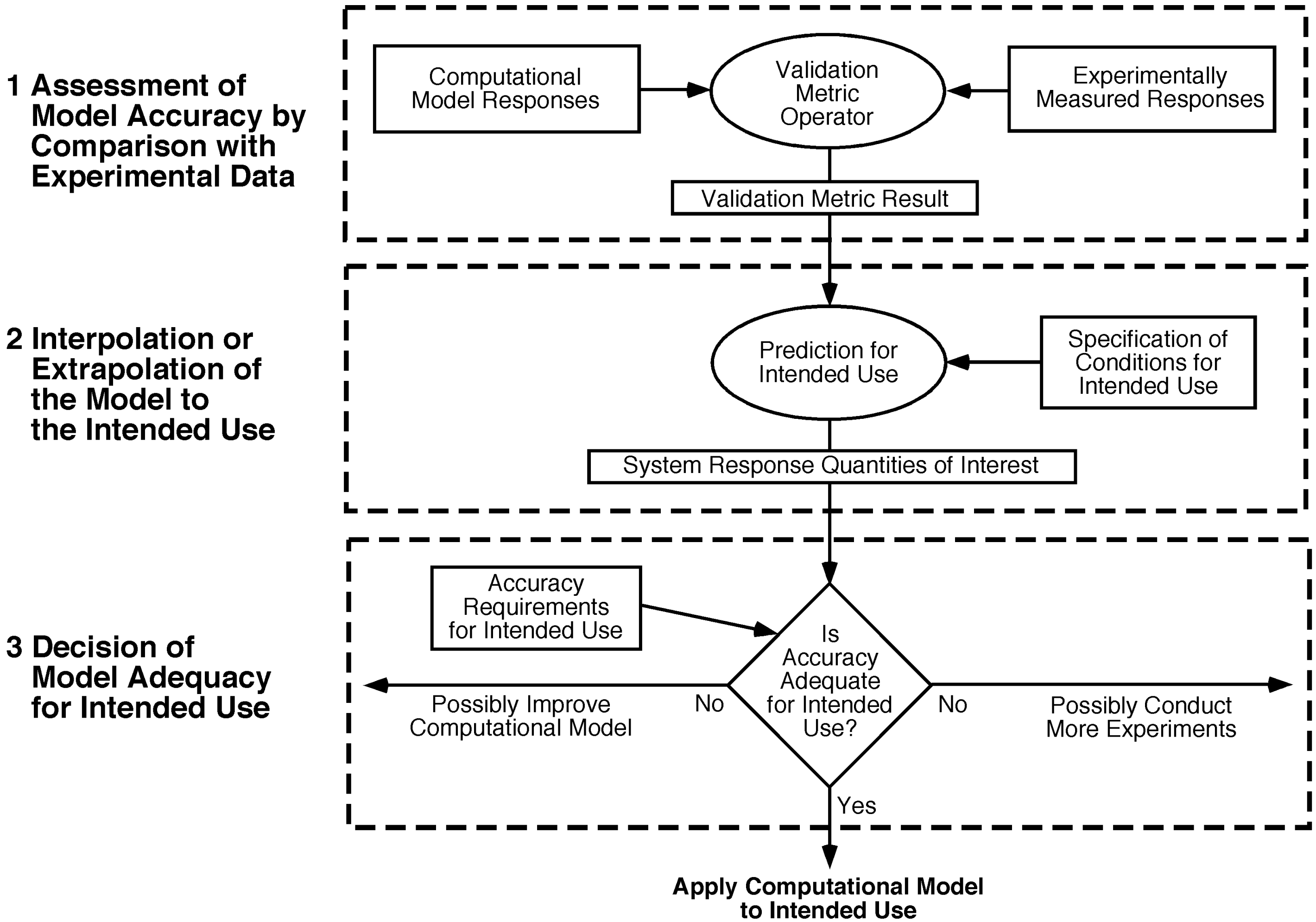
Strategy: Reduce as much as possible

- **Computational model uncertainties and errors**
- **Random (precision) errors and bias (systematic) errors in the experiment**
- **Incomplete physical characterization of the experiment**

Code and solution verification should be performed

before validation activities to be meaningful

Three Aspects of Validation and Prediction



(Ref: Oberkampf and Trucano, 2008)

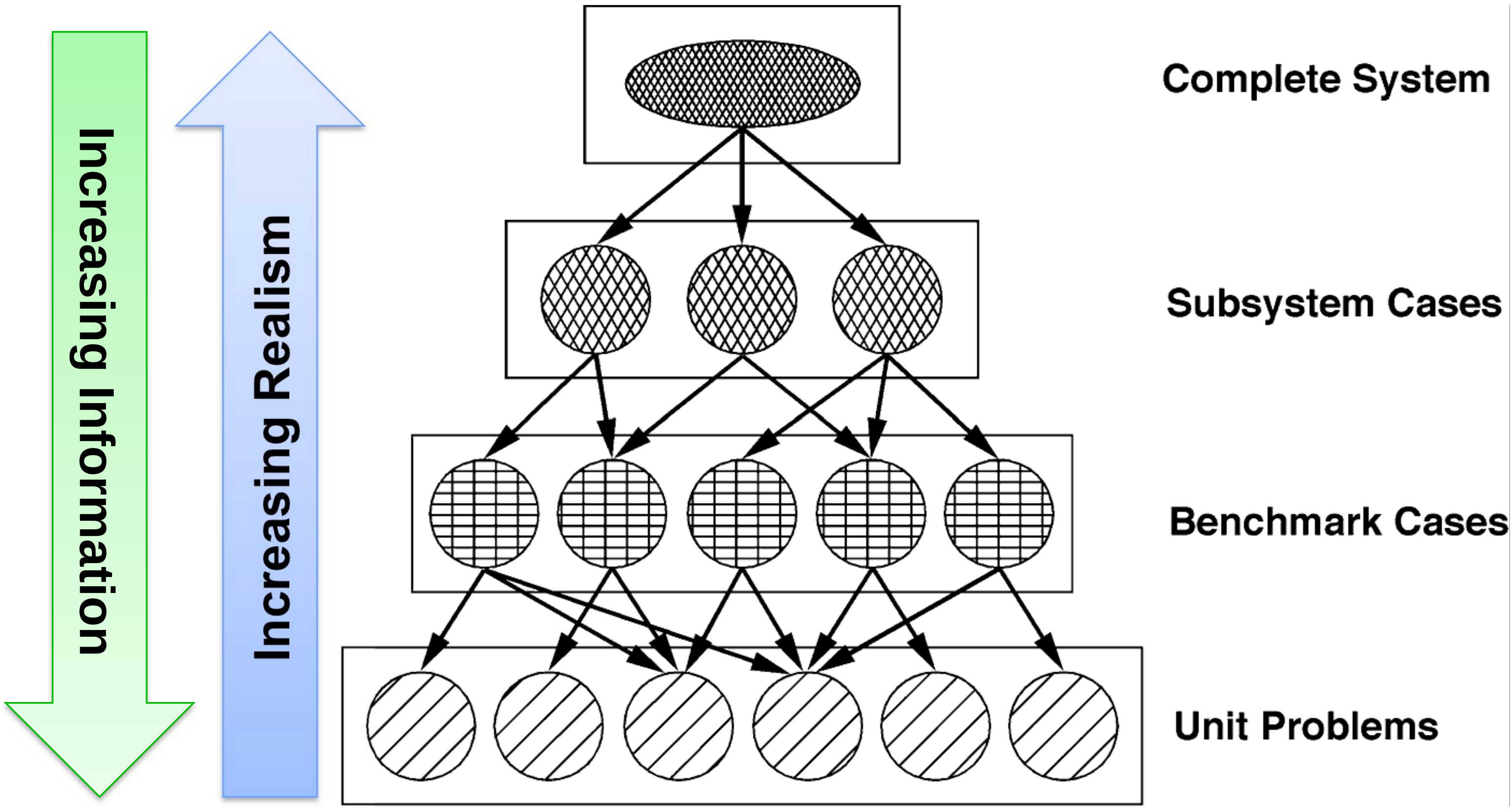
Traditional Experiments vs. Validation Experiments

Three types of traditional experiments:

1. **Improve the fundamental understanding of the physics:**
   - **Ex: Fluid dynamic turbulence experiment; experiment for understanding the decomposition of a thermal protection material**
2. **Improve the mathematical models of some physical phenomena:**
   - **Ex: Model calibration experiment for detonation chemistry; model calibration experiment for crack propagation in materials**
3. **Assess subsystem or complete system performance:**
   - **Ex: Performance of a rocket engine turbopump; performance of a solid-fueled rocket motor**

- **Model validation experiment**
  - **An experiment that is designed and executed to quantitatively estimate a mathematical model's ability to simulate a physical system or process.**
- **The computational model developer or code user is the customer.**

Validation Experiment Hierarchy



(Ref: AIAA Guide, 1998)

Concluding Remarks

- Traditional software quality practices are helpful, but they have been shown to be ineffective in eliminating programming errors (Hatton, 1997)
- The Method of Manufactured Solutions has proven to be very effective, but more solutions are needed in various fields
- Obtaining convergence in the asymptotic region has proven to be difficult, especially on complex problems
- How much code and solution verification is enough?
- Calibration and validation of models have different goals
- Experience has shown that even at lower levels in the validation hierarchy, models do not agree well with data

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